

5. SOIL ALGORITHMS

In this chapter, the T-factors for the transport and transformation of chemical species within and among soil compartments, including the ground-water stratum, are described. In addition, algorithms for the transport of a chemical between soil compartments and the lower atmosphere and between soil compartments and surface water are presented. The text box on the next page and continued on the following pages provides a summary of the T-factor algorithms developed in this chapter and defines all parameters used in those algorithms.

The remainder of this chapter is divided into five subsections. The first outlines the four soil compartment types and the general transport processes that apply to each (Section 5.1). The next (Section 5.2) describes the transformation and degradation processes that apply to the soil compartments. The third subsection develops the T-factor algorithms for vertical-transport between compartments (Section 5.3), while the fourth subsection describes the horizontal-transport algorithms that apply to the surface soil compartments (Section 5.4). Finally, the algorithms related to the ground-water compartment are described (Section 5.5).

5.1 SOIL COMPARTMENTS AND TRANSPORT PROCESSES

In TRIM.FaTE, soil is modeled as four distinct compartment types: surface soil, plant root-zone soil, vadose-zone soil above the saturated zone, and the saturated zone or ground water. In TRIM.FaTE, the root-zone and vadose-zone soils can be sub-divided into one or more vertically stacked compartments for the purpose of assessing mass transfer. Tables 5-1 and 5-2 summarize the gains and losses for surface and subsurface soil compartments, respectively, that are addressed in the current TRIM.FaTE library.

As indicated in Table 5-1, the uppermost surface soil compartment exchanges mass with the lowest compartment of the atmosphere by a combination of diffusion and advection processes. There are two advective processes addressed in TRIM.FaTE that can potentially transport a chemical from a surface soil compartment to down-gradient surface soil compartments or to surface water: erosion of surface soil particles and runoff of water from surface soil. Erosion applies to the solid phase, while runoff and recharge apply to the dissolved phase.

As indicated in Table 5-2, two of the primary transport processes in subsurface soils are exchanges by diffusion and advection. Transport can occur both in the gas and liquid phases. The predominant transport mechanism in the aqueous phase is advection, and that in the gas phase is diffusion. The advective transport of contaminants in the liquid or gas phase depends on the velocity of that phase. There currently is only one advective process included in the TRIM.FaTE library that can potentially transport a chemical from the vadose-zone soil compartment to ground water, that is percolation. Recharge of ground water to surface water also is included. Important physicochemical properties include solubility, molecular weight, vapor pressure, and diffusion coefficients in air and water. The important landscape properties include temperatures of air, rainfall rates, soil properties (*i.e.*, bulk density, porosity), and the depth of each soil compartment.

Summary of Transfer Factors for Soil in TRIM.FaTE

VERTICAL EXCHANGES BETWEEN SURFACE SOIL AND ATMOSPHERE

Diffusion of vapor-phase from air to surface soil: (TF 5-1)

$$T_{Ss \rightarrow Air}^{dif} = \frac{f_A \times A_{Ss}}{Z_{Total_Ss} \times V_{Ss}} \times \left(\frac{1}{Z_{pure_air} \times U_{Air}} + \frac{1}{Z_{Total_Ss} \times U_{Ss}} \right)^{-1}$$

Diffusion of vapor-phase from surface soil to air: (TF 5-2)

$$T_{Air \rightarrow Ss}^{dif} = \frac{f_A \times A_{Ss}}{Z_{Total_Air} \times V_{Air}} \times \left(\frac{1}{Z_{pure_air} \times U_{Air}} + \frac{1}{Z_{Total_Ss} \times U_{Ss}} \right)^{-1}$$

Dry deposition of particle-phase from air to surface soil: (TF 5-3b) ^a

$$T_{AirP \rightarrow Ss}^{dry_dep} = \frac{v_{dry} \times (1 - I_{dry}) \times A_{Ss}}{V_{Air}} \times f_{MS}$$

Wet deposition of particle-phase from air to surface soil during rain: (TF 5-4)

$$T_{AirP \rightarrow Ss}^{wet_dep} = \frac{v_{wet} \times (1 - I_{wet}) \times A_{Ss}}{V_{Air}} \times f_{MS}$$

Wet deposition of vapor-phase from air to surface soil during rain (fugacity approach): (TF 5-5a)

$$T_{Air \rightarrow Ss}^{Vwet_dep} = \frac{A_{Ss}}{V_{Air}} \times rain \times (1 - I_{wet}) \times \frac{Z_{pure_water}}{Z_{Total_Air}}$$

Wet deposition of vapor-phase from air to surface soil during rain (partitioning approach): (TF 5-5b)

$$T_{Air \rightarrow Leaf}^{Vwet_dep} = \frac{A_{Ss}}{V_{Air}} \times w_{rV} \times rain \times (1 - I_{wet}) \times f_{MV}$$

Dry resuspension of particle-phase to air from surface soil compartment: (TF 5-6)

$$T_{Ss \rightarrow AirP}^{res} = \frac{A_{Ss}}{V_{Ss}} \times \frac{res}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Ss}}$$

^a TF 5-5a represents the same basic equation, but uses the fugacity notation. TF 5-5b is the expression of the equation in the current TRIM.FaTE library.

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

VERTICAL EXCHANGES BETWEEN SOIL COMPARTMENTS

Diffusion downward from soil compartment i to the soil compartment j directly below it: (TF 5-7)

$$T_{Si \rightarrow Sj}^{dif} = \frac{Y_{Sij}}{d_{Si} \times Z_{Total_Si}}$$

Diffusion upward from soil compartment j to the soil compartment i immediately above it: (TF 5-8)

$$T_{Sj \rightarrow Si}^{dif} = \frac{Y_{Sij}}{d_{Sj} \times Z_{Total_Sj}}$$

Percolation downward from soil compartment i to soil compartment j : (TF 5-9)

$$T_{Si \rightarrow Sj}^{perc} = \frac{ve_{Si} \times \gamma_{Si}}{(e^{\gamma_{Si} \times d_{Si}} - 1)}$$

HORIZONTAL EXCHANGES ACROSS SURFACE SOIL COMPARTMENTS

Runoff during rain from surface soil compartment i to surface soil compartment j : (TF 5-10a)

$$T_{Ssi \rightarrow Ssj}^{runoff} = runoff \times f_{runoff}(Ssi \rightarrow Ssj) \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML}$$

Erosion during rain from surface soil compartment i to surface soil compartment j : (TF 5-11a)

$$T_{Ssi \rightarrow Ssj}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow Ssj) \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P}$$

Runoff during rain from surface soil compartment i to surface soil sink, same as TF 5-10a but with Ss_sink replacing Ssj : (TF 5-10c)

Erosion during rain from surface soil compartment i to surface soil sink, same as TF 5-11a but with Ss_sink replacing Ssj : (TF 5-11c)

HORIZONTAL TRANSFER FROM SURFACE SOIL TO SURFACE WATER

Runoff during rain from surface soil compartment i to surface water compartment: (TF 5-10b)

$$T_{Ssi \rightarrow SW}^{runoff} = runoff \times f_{runoff}(Ssi \rightarrow SW) \times f_{avail_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML}$$

Erosion during rain from surface soil compartment i to surface water compartment: (TF 5-11b)

$$T_{Ssi \rightarrow SW}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow SW) \times f_{avail_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P}$$

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

VERTICAL EXCHANGES WITH GROUND WATER

Percolation from vadose-zone soil to ground water: (TF 5-12)

$$T_{Sv \rightarrow GW} = \frac{ve_{Sv} \times \gamma_{Sv}}{(e^{\gamma_{Sv} \times d_{Sv}} - 1)}$$

Recharge from ground water to surface water: (TF 5-13)

$$T_{GW \rightarrow SW} = \frac{A_{SWG W}}{V_{GW}} \times \frac{Z_{pure_water}}{Z_{Total_GW}} \times recharge$$

LIST OF SYMBOLS USED IN TRANSFER FACTOR ALGORITHMS

f_A	=	fraction of area available for vertical diffusion (from 0 to 1.0);
A_{Ss}	=	horizontal area of the surface soil compartment (m ²). (This is the area assumed to be shared between the top soil compartment and the atmosphere.)
Z_{Total_Ss}	=	total fugacity capacity of surface soil compartment (mol/m ³ -Pa).
V_{Ss}	=	volume of surface soil compartment (m ³).
Z_{pure_air}	=	fugacity capacity of chemical in pure air, = 1/RT (mol/m ³ -Pa).
U_{Air}	=	mass transfer coefficient on the air side of the air/soil boundary (m/day). (It is typical to represent the mass transfer coefficient in air as the ratio of the diffusion coefficient in air, D_{air} , divided by the turbulent boundary compartment thickness, δ_{air} . For many compounds, D_{air} is on the order of 0.4 m/day and δ_{air} is on the order of 0.0005 m, so that U_{air} is on the order of 800 m/day.)
V_{Air}	=	volume of the air compartment (m ³).
Z_{Total_Air}	=	total fugacity capacity of chemical in the air compartment (includes gas and particle phase of the atmosphere) (mol/m ³ -Pa).
u_{dry}	=	volumetric dry particle deposition rate (m ³ [dust particles]/m ² [surface water]-day).
I_{dry}	=	fraction of dry particle deposition that is intercepted by plants (unitless).
f_{MS}	=	fraction of total chemical mass in compartment that is sorbed to solid particles divided by volume fraction of the compartment that consists of particles (unitless).
u_{wet}	=	volumetric wet particle deposition rate (m ³ [dust particles]/m ² [surface water]-day).
I_{wet}	=	fraction of wet particle deposition that is intercepted by plants (unitless).
$rain$	=	rate of rainfall (m ³ [rain]/m ² [surface soil]-day).
Z_{pure_water}	=	fugacity capacity of chemical in the moving phase, water (mol/m ³ -Pa).
w_{rV}	=	vapor washout ratio (g[chemical dissolved]/m ³ [rain] per g[chemical vapor-phase]/m ³ [air]).
f_{MV}	=	fraction chemical mass in air compartment that is in vapor-phase divided by the volume fraction of air compartment that is gas (unitless).
res	=	rate of resuspension of dust particles from soil to air (kg[dust particles]/m ² [surface soil]-day).
ρ_p	=	density of dust or soil particles in air (kg[particles]/m ³ [particles]).
Z_{pure_solid}	=	fugacity capacity of chemical in the moving phase, dust particles (mol/m ³ -Pa).
γ_{Si}	=	gradient of soil concentration change in soil compartment i (/m).
d_{Si}	=	thickness of surface soil compartment i (m).
Y_{Sij}	=	fugacity-capacity adjusted mass transfer coefficient between soil compartments i and j (mol/m ² -Pa-day), and is given by:

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN TRANSFER FACTOR ALGORITHMS (cont.)

$$Y_{Sij} = \frac{(Z_{Total_Si} \times De_{Si} \times \gamma_{Si}) + (Z_{Total_Sj} \times De_{Sj} \times \gamma_{Sj})}{2 \times \left[\frac{(e^{+\gamma_{Si} \times d_{Si}} - 1)}{\gamma_{Si} \times d_{Si}} - \frac{(1 - e^{-\gamma_{Si} \times d_{Si}})}{\gamma_{Sj} \times d_{Sj}} \right]}$$

d_{Si}, d_{Sj}	=	thickness of soil compartments i and j , respectively (m).
Z_{Total_Si}	=	total fugacity capacity of chemical in soil compartment i (mol/m ³ -Pa).
Z_{Total_Sj}	=	total fugacity capacity of chemical in soil compartment j (mol/m ³ -Pa).
γ_{Si}, γ_{Sj}	=	gradient of soil concentration change in soil compartments i and j , respectively (/m).
De_{Si}	=	effective diffusion coefficient in soil compartment i (m ² [soil]/day).
ve_i	=	effective advection velocity of a chemical in the soil compartment i (m/day), and equal to the rate of soil-solution movement, v_i (see below), multiplied by the fugacity capacity of the moving phase (water) divided by the total fugacity capacity of the soil compartment i ; $ve_i = (v_i \times Z_{pure_water})/Z_{Total_Si}$
v_i	=	average velocity of the moving phase (assumed to be water) in soil compartment i (/m).
$runoff$	=	flux of water transported away from surface soil compartment i (m ³ [water]/m ² [soil]-day).
$f_{runoff}(Ssi \rightarrow Ssj)$	=	fraction of water that runs off of surface soil compartment i that is transported to surface soil compartment j (unitless).
f_{avail_runoff}	=	fraction of surface soil available for runoff (between 0 and 1.0).
f_{ML}	=	fraction of chemical in compartment that is dissolved in water divided by the volume fraction of the compartment that is liquid (water).
$erosion$	=	flux of soil particles transported away from surface soil compartment i (kg[soil particles]/m ² [soil]-day).
$f_{erosion}(Ssi \rightarrow Ssj)$	=	fraction of soil that erodes from surface soil compartment i that is transported to surface soil compartment j (unitless).
$f_{avail_erosion}$	=	fraction of surface soil available for erosion (between 0 and 1.0).
ve_{Sv}	=	effective advection velocity of a chemical in the vadose-zone soil compartment (m/day).
γ_{Sv}	=	gradient of soil concentration change in vadose-zone soil compartment (/m).
A_{SWGw}	=	interfacial area between ground-water and surface-water compartments (m ²).
V_{GW}	=	volume of ground-water compartment (m ³).
Z_{Total_GW}	=	total fugacity of chemical in the ground-water compartment (mol/m ³ -Pa).
$recharge$	=	average daily recharge from ground water into surface water (m/day).

A future version of the TRIM.FaTE library could include algorithms for diffusive transfers between the vadose-zone soil compartment and the ground-water compartment.

5.2 TRANSFORMATIONS AND DEGRADATION

The transformation of chemicals in soil layers can have a profound effect on their potential for persistence. Chemical transformations, which may occur as a result of biotic or abiotic processes, can significantly reduce the concentration of a substance in soil.

Table 5-1
Summary of the Chemical Gains and Losses for Surface Soil
Compartments Addressed in TRIM.FaTE

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Air			To Air		
Diffusion from air	Diffusion (TF 5-1)	Vapor	Diffusion to air	Diffusion (TF5-2)	Vapor
Dry deposition of particles/ aerosols from air	Advection (TF 5-3)	Solid	Dry resuspension of particle phase	Advection (TF 5-6)	Solid
Wet deposition of particles/ aerosols from air	Advection (TF 5-4)	Solid			
Wet deposition of vapor from air	Advection (TF 5-5)	Vapor			
From Surface Soils			To Surface Soils		
Erosion from upgradient soils	Advection (TF 5-10a)	Solid	Erosion to downgradient soils	Advection (TF 5-10a)	Solid
Runoff from upgradient soils	Advection (TF 5-11a)	Aqueous	Runoff to downgradient soils	Advection (TF 5-11a)	Aqueous
From Plants			To Plants		
Deposition of leaves during litter fall	Advection (TF 7-15)	Solid			
Deposition of particles on leaves during litter fall	Advection (TF 7-16)	Solid			
From Surface Water			To Surface Water		
			Erosion	Advection (TF 5-11b)	Solid
			Runoff	Advection (TF 5-10b)	Aqueous
From Terrestrial Birds and Mammals			To Terrestrial Birds and Mammals		
Elimination from terrestrial and semi-aquatic wildlife	Advection (TF 7-31)	Total	Ingestion by wildlife	Advection (TF 7-22)	Total
From Root-Zone Soil			To Root-Zone Soil		
Upward diffusion	Diffusion (TF 5-8)	Aqueous & Vapor	Percolation	Advection (TF 5-9)	Aqueous
			Diffusion	Diffusion (TF 5-7)	Aqueous & Vapor
From Surface Soil Transformations			To Sink(s)		
			Runoff off-site to sink	Advection (TF 5-10c)	Aqueous
			Erosion off-site to sink	Advection (TF 5-11c)	Solid
			Decay to reaction sinks	Degradation (TF 2-1)	Total

Table 5-2
Summary of the Chemical Gains and Losses for Sub-surface Soil
Compartment *j* Addressed in TRIM.FaTE^a

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Vertically Adjacent Soil Compartment			To Vertically Adjacent Soil Compartment		
Downward diffusion from soil compartment <i>i</i>	Diffusion (TF 5-7)	Aqueous	Downward diffusion from soil compartment <i>j</i>	Diffusion (TF 5-7)	Aqueous
Upward diffusion from soil compartment <i>l</i>	Diffusion (TF 5-8)	Aqueous	Upward diffusion from soil compartment <i>j</i>	Diffusion (TF 5-8)	Aqueous
Percolation downward from soil compartment <i>i</i>	Advection (TF 5-9)	Aqueous	Percolation downward from soil compartment <i>j</i>	Advection (TF 5-9)	Aqueous
			To Plants		
Release from plant roots	Diffusion (TF 7-11)		Uptake from root-zone soil by plant roots	Diffusion (TF 7-10)	Aqueous
			Uptake by plant stems from root-zone soil via flow of transpired water	Advection (TF 7-12a)	Aqueous
From Ground Water			To Ground Water		
			Percolation from vadose-zone soil	Advection (TF 5-12)	Aqueous
From Surface Water			To Surface Water		
			Recharge from ground water	Advection (TF 5-13)	Aqueous
From Soil Transformations			To Sink(s)		
			Decay to reaction sinks	Degradation (TF 2-1)	Total

^aSub-surface soil compartment *i* is higher than *j* is higher than *l*.

Transformations of chemicals into compounds that will no longer be tracked in TRIM.FaTE (*e.g.*, non-toxic degradation products) are called general degradation processes in the model. In TRIM.FaTE, the degradation of chemicals in soil due to all mechanisms that might apply (*e.g.*, degradation by soil microfauna, photolysis at the soil surface, hydrolysis in the saturated zone) is reflected by the user input for the half-life of the chemical in the particular soil compartment. The algorithm relating the degradation rate constant to the chemical half-life in a soil compartment is presented in Chapter 2 (Equation 2-64).

Transformations of a chemical into another form of the chemical that is tracked in TRIM.FaTE are reflected in algorithms that are named for the process (*e.g.*, oxidation, methylation, reduction of mercury species). In the TRIM.FaTE soil layers, all transformation processes are modeled as first-order processes, that is, linear with inventory (*i.e.*, the quantity of chemical contained in a compartment). The rate of mass removal in a first-order transformation is calculated as the product of the total inventory and the transformation rate constant. The transformation rate constant is the inverse of the residence time with respect to that reaction.

5.3 VERTICAL TRANSPORT ALGORITHMS

The transfer factors in the subsurface are a function of the advective flux (gas phase plus liquid phase) and the diffusive flux (gas phase plus liquid phase). In the subsections below, upward and downward transfer factors are developed for the top three soil compartments (*i.e.*, excluding ground water). No provisions are made for preferential flow regions in the vadose zone that could lead to higher concentrations in the ground water, because in most cases, the proportion of exposure from ground water is minimal for air pollutants.

5.3.1 THEORETICAL BASIS FOR THE TRANSPORT ALGORITHMS

The algorithms below are developed by assuming that chemical concentration in each compartment decreases exponentially with depth in that compartment. This type of concentration gradient has been demonstrated as the correct analytical solution of the one-dimensional, convective-dispersive, solute-transport equation in a vertical layer with a steady-state concentration maintained at its upper surface (ARS 1982). With the assumption of exponentially decreasing vertical concentration for each soil compartment, *i*, the variation in concentration with depth in that compartment is given by:

$$C_i(x) = C_i(0) \times \exp(-\gamma_i x) \quad (\text{Eq. 5-1})$$

where:

- x = distance into the soil compartment measured from the top of the soil column (m);
- $C_i(0)$ = peak chemical concentration in soil compartment *i* (g[chemical]/m³[soil]), which is related to the total inventory N_i (g[chemical]) in this soil compartment (this relationship is provided below); and
- γ_i = the gradient of soil concentration change in soil compartment *i* (/m), which is obtained from the inverse of the normalized or characteristic depth X^* , which is $\gamma_i = 1/X^*$.

X^* can be input by the user. If the user does not provide a value, a value for X^* is calculated as follows. Let:

- λ_i = removal rate constant for a chemical in soil compartment *i*, based on chemical transformation (/day); then

$$\begin{aligned} \text{If } \lambda_i > 0 \text{ then } X^* &= \text{Minimum } (DX_1, DX_2), \\ \text{Otherwise (i.e., } \lambda_i &= 0), \text{ then } X^* = DX_2. \end{aligned} \quad (\text{Eq. 5-2})$$

DX_i is the Damkoehler distance (the distance at which the soil concentration falls by 1/e based on the aggregate results of diffusion, advection, and reaction) in units of meters and is given by:

$$DX_1 = \frac{ve_i + \sqrt{ve_i^2 + 4De_{Si}}}{2\lambda_i} \quad (\text{Eq. 5-3a})$$

Equation 5-3a can be rearranged as follows to arrive at Equation 5-3d, which is the form of the equation in the TRIM.FaTE library:

$$DX_1 = \frac{ve_i}{2\lambda_i} + \frac{\sqrt{(ve_i)^2 + (4De_{Si} \times \lambda_i)}}{2\lambda_i} \quad (\text{Eq. 5-3b})$$

$$DX_1 = \frac{ve_i}{2\lambda_i} + \sqrt{\frac{(ve_i)^2}{4\lambda_i^2} + \left(\frac{4De_{Si} \times \lambda_i}{4\lambda_i^2}\right)} \quad (\text{Eq. 5-3c})$$

$$DX_1 = \frac{ve_i}{2\lambda_i} + \sqrt{\left(\frac{ve_i}{2\lambda_i}\right)^2 + \left(\frac{De_{Si}}{\lambda_i}\right)} \quad (\text{Eq. 5-3d})$$

If $ve_i = 0$, then:

$$DX_1 = \sqrt{\frac{De_{Si}}{\lambda_i}} \quad (\text{Eq. 5-3e})$$

In Equations 5-3a through 5-3e, the following parameter definitions apply:

De_{Si} = effective diffusion coefficient in soil compartment i ($\text{m}^2[\text{soil}]/\text{day}$), which is derived below in Equation 5-7; and
 ve_i = the effective advection velocity of a chemical in the soil compartment, i (m/day), and equal to the rate of soil-solution movement, v_i , multiplied by the fugacity capacity of the moving phase and divided by the fugacity capacity of soil compartment i :

$$ve_i = (v_i \times Z_{\text{pure_water}}) / Z_{\text{Total_Si}} \quad (\text{Eq. 5-4})$$

where:

v_i = average velocity of the moving liquid phase (assumed to be water) in the soil column i (m/day);
 $Z_{\text{pure_water}}$ = fugacity capacity of chemical in the moving phase, water ($\text{mol}/\text{m}^3\text{-Pa}$); and
 $Z_{\text{Total_Si}}$ = total fugacity capacity of chemical in soil compartment i ($\text{mol}/\text{m}^3\text{-Pa}$).

DX_2 is the depth that establishes the concentration gradient in soil in the absence of any reaction or transformation processes, in units of meters. It is obtained as follows:

$$\begin{aligned} \text{If } ve_i > 0, \text{ then } DX_2 &= \text{Minimum} [(4 \times De_i / ve_i), (2d_i \times \sqrt{\pi})] \\ \text{Otherwise (i.e., } ve_i &= 0), DX_2 = (2d_i \times \sqrt{\pi}) \end{aligned} \quad (\text{Eq. 5-5})$$

where:

d_i = the thickness of soil compartment i (m).

As an average, the property v_i (m/day), the average velocity of the moving liquid phase (assumed to be water) in the soil column i , is intended to be representative of the range of velocities occurring, and not be limited only to the velocity during rainfall events. The user should check that the value used for v_i in the TRIM.FaTE library is consistent with the precipitation data in the scenario (adjusted for infiltration) (see the TRIM.FaTE user guidance).

Compartments such as soils and sediments are neither homogeneous nor single phase. When air and water occupy the tortuous pathways between stationary particles in a porous medium such as a soil or sediment, Millington and Quirk (1961) have shown that the effective diffusivity is given by:

$$De = (\omega^{10/3} / \phi^2) \times D_{\text{pure}} \quad (\text{Eq. 5-6})$$

where:

De = effective diffusivity of a chemical in either the air or water phase of the mixture ($\text{m}^2[\text{fluid}]/\text{day}$);
 ω = volume fraction occupied by that fluid (either air or water) (unitless);
 ϕ = porosity or total void fraction in the medium (the volume occupied by all fluids) (unitless); and
 D_{pure} = diffusion coefficient of the chemical in the pure fluid ($\text{m}^2[\text{fluid}]/\text{day}$).

Jury et al. (1983) have shown that the effective tortuous diffusivity in the water and air of a soil compartment i , such as the root-zone soil(s), is given by:

$$De_{Si} = \frac{Z_{\text{pure_air}}}{Z_{\text{Total_Si}}} \times (\epsilon_i^{10/3} / \phi_i^2) \times D_{\text{air}} + \frac{Z_{\text{pure_water}}}{Z_{\text{Total_Si}}} \times (\theta_i^{10/3} / \phi_i^2) \times D_{\text{water}} \quad (\text{Eq. 5-7})$$

where:

De_{Si} = the effective tortuous, mixed-phase diffusion coefficient in the soil compartment i ($\text{m}^2[\text{soil}]/\text{day}$);
 ϵ_i = volume fraction of soil compartment i that is air (unitless);
 θ_i = volume fraction of soil compartment i that is water (unitless);
 $Z_{\text{pure_air}}$ = fugacity capacity of chemical in the gas-phase of air ($\text{mol}/\text{m}^3\text{-Pa}$);
 $Z_{\text{pure_water}}$ = fugacity capacity of chemical in the soil water ($\text{mol}/\text{m}^3\text{-Pa}$);
 $Z_{\text{Total_Si}}$ = total fugacity capacity of chemical in soil compartment i ($\text{mol}/\text{m}^3\text{-Pa}$);
 D_{air} = the diffusion coefficient of the chemical in air (excluding atmospheric dust particulates) ($\text{m}^2[\text{air}]/\text{day}$); and

D_{water} = the diffusion coefficient of the chemical in water (excluding suspended sediments (m^2 [water]/day)).

5.3.2 RELATIONSHIP BETWEEN INVENTORY, N_{Si} , AND PEAK CONCENTRATION, $C_{Si}(0)$

The assumptions of a peak chemical concentration and an exponential gradient of chemical concentration within a soil compartment make it possible to define $C_{Si}(0)$ in terms of the inventory, N_{Si} :

$$N_{Si} = A_{Si} \times \int_0^{d_{Si}} C_{Si}(0) \times \exp(-\gamma_{Si} x) dx \quad (\text{Eq. 5-8})$$

$$N_{Si} = A_{Si} \times [C_{Si}(0) / \gamma_{Si}] \times [1 - \exp(-\gamma_{Si} \times d_{Si})] \quad (\text{Eq. 5-9})$$

where:

N_{Si} = inventory of chemical in soil compartment i (g[chemical]);
 A_{Si} = horizontal area of the soil compartment i (m^2);
 C_{Si} = chemical concentration in soil compartment i (g[chemical]/ m^3 [soil]);
 γ_{Si} = the gradient of soil concentration change in soil compartment i (/m) (see Equation 5-1); and
 d_{Si} = thickness of soil compartment i (m).

Solving Equation 5-9 for $C_{Si}(0)$ yields:

$$C_{Si}(0) = \frac{N_{Si} \times \gamma_{Si}}{A_{Si} \times [1 - \exp(-\gamma_{Si} \times d_{Si})]} \quad (\text{Eq. 5-10})$$

5.3.3 VERTICAL MASS EXCHANGE BETWEEN AIR AND THE SURFACE SOIL COMPARTMENT

Both diffusive and advective processes can transfer a chemical between the air and the surface soil compartment. The diffusive process can result in a two-way exchange of vapor-phase chemical between the surface soil and air above it (Section 5.3.3.1). The advective processes are one-way, from air to surface soil. These include the wet and dry deposition of particle-bound chemical (*i.e.*, solid phase) (Section 5.3.3.2) and the wet deposition of vapor-phase chemical scavenged from the air during rain.

5.3.3.1 Diffusive Processes

The algorithm for representing diffusion exchange at the air/soil interface is based on defining the flux from air to soil in terms of the concentration gradient at the point of contact between air and soil (Eq. 5-11) and the flux from soil to air in terms of the bulk chemical concentration in the surface soil layer (Eq. 5-12):

$$Flux (air\ side) = U_{Air} \times \left[C_{Air} - C_{Ss}(0) \times \frac{Z_{pure_air}}{Z_{Total_Ss}} \right] \quad (Eq. 5-11)$$

$$Flux (soil\ side) = U_{Ss} \times [C_{Ss}(0) - C_{Ss}] \quad (Eq. 5-12)$$

where:

- $Flux$ = transfer rate per unit area (g[chemical]/m²[air/soil interface]-day);
- U_{Air} = mass-transfer coefficient on the air side of the air/soil interface (m/day) (It is typical to represent the mass transfer coefficient in air as the ratio of the diffusion coefficient in air, D_{air} , divided by the turbulent boundary compartment thickness, δ_{air} . For many compounds, D_{air} is on the order of 0.4 m/day, and δ_{air} is on the order of 0.0005 m, so that U_{Air} is on the order of 800 m/day.);
- C_{Air} = concentration of the chemical in the gas phase of the lowest compartment of the atmosphere (g[chemical]/m³[gas-phase air]), derived in Equation 5-16 below;
- $C_{Ss}(0)$ = chemical concentration at the top of the uppermost (*i.e.*, surface) soil compartment in a vertical set of soil compartments (g[chemical]/m³[soil]), as given for $C_i(0)$ in Equation 5-10;
- Z_{pure_air} = fugacity capacity of chemical in air, = 1/RT (mol/m³-Pa);
- Z_{Total_Ss} = total fugacity capacity of chemical in surface soil compartment (mol/m³-Pa);
- U_{Ss} = mass-transfer coefficient on the soil side of the air/soil interface (m/day); and
- $C_{Ss}(bulk)$ = total chemical concentration in bulk surface soil (g[chemical]/ m³[soil]).

Rearranging Equations 5-11 and 5-12 yields Equations 5-13 and 5-14, respectively:

$$\frac{Flux}{Z_{pure_air} \times U_{Air}} = \left[\frac{C_{Air}}{Z_{pure_air}} - \frac{C_{Ss}(0)}{Z_{Total_Ss}} \right] \quad (Eq. 5-13)$$

$$\frac{Flux}{Z_{Total_Ss} \times U_{Ss}} = \left[\frac{C_{Ss}(0)}{Z_{Total_Ss}} - \frac{C_{Ss}(bulk)}{Z_{Total_Ss}} \right] \quad (Eq. 5-14)$$

Adding Equations 5-13 and 5-14 together yields:

$$Flux \times \left[\frac{1}{Z_{pure_air} \times U_{Air}} + \frac{1}{Z_{Total_Ss} \times U_{Ss}} \right] = \left[\frac{C_{Air}}{Z_{pure_air}} - \frac{C_{Ss}(bulk)}{Z_{Total_Ss}} \right] \quad (\text{Eq. 5-15})$$

$$Flux = \left[\frac{C_{Air}}{Z_{pure_air}} - \frac{C_{Ss}(bulk)}{Z_{Total_Ss}} \right] \times \left[\frac{1}{Z_{pure_air} \times U_{Air}} + \frac{1}{Z_{Total_Ss} \times U_{Ss}} \right]^{-1} \quad (\text{Eq. 5-16})$$

The bulk concentration of the chemical in the lowest compartment of the atmosphere is given by:

$$C_{Air} = \frac{N_{Air} \times Z_{pure_air}}{V_{Air} \times Z_{Total_Air}} \quad (\text{Eq. 5-17})$$

where:

$$\begin{aligned} N_{Air} &= \text{inventory of chemical in the air compartment above the soil (g[chemical]);} \\ Z_{pure_air} &= \text{fugacity capacity of chemical in gas-phase air (mol/m}^3\text{-Pa);} \\ V_{Air} &= \text{volume of the air compartment (m}^3\text{[air]); and} \\ Z_{Total_Air} &= \text{total fugacity capacity of chemical in air compartment (including gas and} \\ &\quad \text{particle phases of the air) (mol/m}^3\text{-Pa).} \end{aligned}$$

The bulk concentration of the chemical in the surface soil layer is given by:

$$C_{Ss} = \frac{N_{Ss}}{V_{Ss}} \quad (\text{Eq. 5-18})$$

where:

$$\begin{aligned} N_{Ss} &= \text{inventory of chemical in the surface soil compartment (g[chemical]); and} \\ V_{Ss} &= \text{volume of the surface soil compartment (m}^3\text{[soil]).} \end{aligned}$$

Finally, the chemical flow between the air and surface soil compartments is determined from the flux and the area of the air/soil interface (as well as the fraction of that area that is not covered by an impervious material):

$$Flow = Flux \times f_A \times A_{Ss} \quad (\text{Eq. 5-19})$$

where:

$$\begin{aligned} Flow &= \text{diffusive flow (g[chemical]/day);} \\ f_A &= \text{fraction of area available for vertical diffusion (unitless, ranges from 0 to} \\ &\quad \text{1); and} \\ A_{Ss} &= \text{area of surface soil compartment (m}^2\text{).} \end{aligned}$$

Making the appropriate substitutions, the net flow of chemical mass between the air and surface soil compartments by diffusion is calculated as:

$$\begin{aligned} \text{Net Diffusion Flow (Air} \leftrightarrow \text{Ss) (g[chemical]/day)} &= (T_{\text{Air} \rightarrow \text{Ss}} \times N_{\text{Air}}) - (T_{\text{Ss} \rightarrow \text{Air}} \times N_{\text{Ss}}) = \\ f_A \times A_{\text{Ss}} \times \left(\frac{N_{\text{Air}}}{Z_{\text{Total_air}} \times V_{\text{Air}}} - \frac{N_{\text{Ss}}}{Z_{\text{Total_Ss}} \times V_{\text{Ss}}} \right) \times \left(\frac{1}{Z_{\text{pure_air}} \times U_{\text{Air}}} + \frac{1}{Z_{\text{Total_Ss}} \times U_{\text{Ss}}} \right)^{-1} \end{aligned} \quad (\text{Eq. 5-20})$$

where:

$Z_{\text{pure_air}}$ = fugacity capacity of chemical in pure air (mol/m³-Pa);
 V_{Air} = volume of the air compartment (m³);
 $Z_{\text{Total_Ss}}$ = total fugacity capacity of chemical in surface soil compartment (mol/m³-Pa);
 V_{Ss} = volume of the surface soil compartment (m³);
 U_{Air} = mass transfer coefficient on the air side of the air/soil boundary (m/day); and
 U_{Ss} = mass transfer coefficient on the soil side of the air/soil boundary (m/day).

This implies the following:

$$T_{\text{Ss} \rightarrow \text{Air}}^{\text{dif}} = \frac{f_A \times A_{\text{Ss}}}{Z_{\text{Total_Ss}} \times V_{\text{Ss}}} \times \left(\frac{1}{Z_{\text{pure_air}} \times U_{\text{Air}}} + \frac{1}{Z_{\text{Total_Ss}} \times U_{\text{Ss}}} \right)^{-1} \quad (\text{TF 5-1})$$

where:

$T_{\text{Ss} \rightarrow \text{Air}}^{\text{dif}}$ = transfer factor for diffusion of chemical from surface soil compartment to air (/day).

It also implies:

$$T_{\text{Air} \rightarrow \text{Ss}}^{\text{dif}} = \frac{f_A \times A_{\text{Ss}}}{Z_{\text{Total_air}} \times V_{\text{Air}}} \times \left(\frac{1}{Z_{\text{pure_air}} \times U_{\text{Air}}} + \frac{1}{Z_{\text{Total_Ss}} \times U_{\text{Ss}}} \right)^{-1} \quad (\text{TF 5-2})$$

where:

$T_{\text{Air} \rightarrow \text{Ss}}^{\text{dif}}$ = transfer factor for diffusion of chemical from air to surface soil compartment (/day).

The mass transfer coefficient for the soil side of the air/soil boundary, U_{Ss} , can be estimated as follows:

$$U_{\text{Ss}} = \frac{De_{\text{Ss}}}{d_{\text{Ss}}} \quad (\text{Eq. 5-21})$$

where :

De_{Ss} = effective diffusion coefficient in surface soil compartment (m²/d) (derived in Equation 5-7); and

d_{ss} = the thickness of the surface soil compartment (m).

It is important to ensure that the area used to calculate the flux, A_{ss} , is the area of the surface soil compartment that is shared with the lowest atmosphere compartment. This is not necessarily the surface area of the lowest atmosphere compartment.

Note: In the current TRIM.FaTE library, these transfer factor algorithms apply to all chemicals except divalent mercury, which is reactive in air. Therefore, a separate algorithm representing net diffusion from air to surface soil is used for divalent mercury (see vapor dry deposition algorithms for Hg(2) described in Appendix A, Section A.1.1).

5.3.3.2 Wet and Dry Deposition of Particles

For wet and dry deposition of particles from air to surface soil, the rate of mass flow is given by:

$$\frac{dN_{ss}}{dt} = \frac{A_{ss}}{V_{Air}} \times v \times (1 - I) \times \frac{D_L}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Air}} \times N_{Air} \quad (\text{Eq. 5-22})$$

where:

N_{ss}	=	inventory of chemical in surface soil compartment (g[chemical]);
A_{ss}	=	area of contact between the surface soil compartment and the lowest air compartment (m ² [soil]);
V_{Air}	=	volume of the air compartment (m ³ [air]);
v	=	air-to-soil deposition velocity, where the velocity is different for wet and dry deposition of particles (m/day);
I	=	fraction of deposition that is intercepted by plants, where the interception fraction is different for wet and dry deposition of particles (unitless);
D_L	=	dust load (<i>i.e.</i> , particulate matter concentration) in air (kg[dust particles]/m ³ [air]);
ρ_P	=	density of dust particles (kg[dust particles]/m ³ [dust particles]);
Z_{pure_solid}	=	fugacity capacity of chemical in dust particles (mol/m ³ -Pa);
Z_{Total_Air}	=	total fugacity capacity of chemical in air compartment (including dust particles) (mol/m ³ -Pa); and
N_{Air}	=	total inventory of chemical in air compartment, vapor- and solid-phase (g[chemical]).

Dry deposition of particle-phase chemical:

Thus, the transfer factor for *dry* deposition of chemical sorbed to air particles to the surface soil is as follows:

$$T_{AirP \rightarrow ss}^{dry_dep} = \frac{A_{ss}}{V_{Air}} \times v_{dry} \times (1 - I_{dry}) \times \frac{D_L}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Air}} \quad (\text{TF 5-3a})$$

where:

$$\begin{aligned} v_{dry} &= \text{air-to-soil dry deposition velocity (m/day); and} \\ I_{dry} &= \text{fraction of dry deposition that is intercepted by plants (unitless) (see Equation 7-2).} \end{aligned}$$

It is also true that:

$$v_{dry} = v_{dry} \times \frac{D_L}{\rho_P} \quad (\text{Same as Eq. 4-1})$$

where:

$$v_{dry} = \text{volumetric dry deposition rate (m}^3\text{[dust]/m}^2\text{[air]-day);}$$

and:

$$\frac{Z_{pure_solid}}{Z_{Total_Air}} = \frac{Mass_Fraction_Sorbed}{Volume_Fraction_Solid} = f_{MS} \quad (\text{Eq. 5-23})$$

where:

$$f_{MS} = \text{mass fraction of the chemical sorbed to solid particles in air divided by the volume fraction of the air compartment that consists of solid particles (unitless) (see Equations 2-71 and 2-79).}$$

Therefore, the transfer factor can be calculated as:

$$T_{AirP \rightarrow Ss}^{dry_dep} = \frac{v_{dry} \times (1 - I_{dry}) \times A_{Ss}}{V_{Air}} \times f_{MS} \quad (\text{TF 5-3b})$$

where:

$$\begin{aligned} T_{AirP \rightarrow Ss}^{dry_dep} &= \text{transfer factor for dry deposition of particulate-bound chemical to surface soil compartment (/day);} \\ v_{dry} &= \text{volumetric dry deposition rate (m}^3\text{[dust]/m}^2\text{[surface soil]-day);} \\ I_{dry} &= \text{fraction of dry deposition that is intercepted by plants (unitless);} \\ A_{Ss} &= \text{area of contact between the surface soil compartment and the lowest air compartment (m}^2\text{); and} \\ V_{Air} &= \text{volume of the air compartment (m}^3\text{[air]).} \end{aligned}$$

Wet deposition of particle-phase chemical:

The transfer factor for wet deposition of particle-phase chemical to the surface soil can be calculated as:

$$T_{AirP \rightarrow Ss}^{wet_dep} = \frac{v_{wet} \times (1 - I_{wet}) \times A_{Ss}}{V_{Air}} \times f_{MS} \quad (\text{TF 5-4})$$

where:

$T_{AirP \rightarrow Ss}^{wet_dep}$	=	transfer factor for wet deposition of particulate-bound chemical to surface soil compartment (/day);
v_{wet}	=	volumetric wet deposition rate ($m^3[dust]/m^2[surface\ soil]-day$);
I_{wet}	=	fraction of wet deposition that is intercepted by plants (unitless) (see Equation 7-4);
A_{Ss}	=	area of contact between the surface soil compartment and the lowest air compartment (m^2);
V_{Air}	=	volume of the air compartment ($m^3[air]$); and
f_{MS}	=	mass fraction of the chemical sorbed to air particles divided by the volume fraction of the air compartment that consists of particles (unitless).

The wet deposition rate is calculated as:

$$v_{wet} = w_r \times rain \times \frac{D_L}{\rho_P} \quad (\text{Same as Eq. 4-5})$$

where:

w_r	=	washout ratio for particles in air ($m^3[air]/m^3[rain]$);
$rain$	=	rate of rainfall (m/day);
D_L	=	dust load (<i>i.e.</i> , particulate matter concentration) in air ($kg[dust\ particles]/m^3[air]$); and
ρ_P	=	density of dust particles ($kg[dust\ particles]/m^3[dust\ particles]$).

5.3.3.3 Wet Deposition of Vapor-phase Chemical

Chemical vapors can be scavenged (absorbed) by the rain water and deposited to the surface soil with the rain. During rain, the advection flow of chemical from air to the upper surface soil compartment is given by:

$$\frac{dN_{Ss}}{dt} = \frac{A_{Ss}}{V_{Air}} \times rain \times (1 - I_{wet}) \times \frac{Z_{pure_water}}{Z_{Total_Air}} \times N_{Air} \quad (\text{Eq. 5-24})$$

where:

N_{Ss}	=	inventory of chemical in the surface soil compartment ($g[chemical]$);
A_{Ss}	=	area of the surface soil compartment ($m^2[soil]$);
$rain$	=	rate of rainfall (m/day);
V_{Air}	=	volume of the air compartment ($m^3[air]$);
Z_{pure_water}	=	fugacity capacity chemical in water (excluding suspended sediments) ($mol/m^3\text{-Pa}$);
Z_{Total_Air}	=	total fugacity capacity of chemical in the air compartment (including dust particles) ($mol/m^3\text{-Pa}$);

I_{wet} = fraction of wet deposition that is intercepted by plants (unitless) (see Equation 7-4); and
 N_{Air} = total chemical inventory in the air compartment, both vapor- and solid-phase (g[chemical]).

Therefore, the transfer factor for wet deposition of vapor-phase chemical to surface soil can be calculated as:

$$T_{Air \rightarrow Ssi}^{Vwet_dep} = \frac{A_{Ss}}{V_{Air}} \times rain \times (1 - I_{wet}) \times \frac{Z_{pure_water}}{Z_{Total_Air}} \quad (TF\ 5-5a)$$

where:

$T_{Air \rightarrow Ssi}^{Vwet_dep}$ = transfer factor for wet vapor deposition from air to surface soil compartment i during a rainfall event (/day).

In the current TRIM.FaTE library, TF 5-5a is used for organic chemicals. For the mercury species, a slightly different algorithm is used:

$$T_{Air \rightarrow Leaf}^{Vwet_dep} = \frac{A_{Ss}}{V_{Air}} \times w_{rV} \times rain \times (1 - I_{wet}) \times f_{MV} \quad (TF\ 5-5b)$$

where:

w_{rV} = vapor washout ratio (g[chemical dissolved]/m³[rain] per g[chemical vapor-phase]/m³[air]) = $1/K_{AW}$, where:
 K_{AW} = air/water partition coefficient (g[chemical]/m³[air] per g[chemical]/m³[water]); and
 f_{MV} = the fraction of the chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the air compartment that is gas/vapor (*i.e.*, fraction that is not particulate) (see Equation 2-81 in Chapter 2).

The derivation of these algorithms is explained in more detail in Chapter 7, Section 7.2.1.6.

5.3.3.4 Dry Resuspension of Dust from Soil to Air

For resuspension of dust from the first surface soil compartment to the lower compartment of the atmosphere, the chemical transfer from soil to air is given by:

$$T_{Ss \rightarrow AirP}^{res} = \frac{A_{Ss}}{V_{Ss}} \times \frac{res}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Ss}} \quad (TF\ 5-6)$$

where:

res	=	rate at which dust particles are resuspended from the soil surface (kg[particles]/m ² [soil surface]-day);
ρ_p	=	density of the dust particles (kg[particles]/m ³ [particles]);
Z_{pure_solid}	=	fugacity capacity of chemical in dust particles (mol/m ³ -Pa); and
Z_{Total_Ss}	=	total fugacity capacity of chemical in surface soil compartment (including dust particles) (mol/m ³ -Pa).

If a value cannot be determined for res , then it can be estimated using the equation:

$$res = v_{dry} \times \rho_p \quad (\text{Eq. 5-25})$$

where:

$$v_{dry} = \text{volumetric dry deposition rate (m}^3\text{[particles]/m}^2\text{[surface soil]-day).}$$

5.3.4 VERTICAL MASS EXCHANGE BETWEEN TWO VERTICALLY ADJACENT SOIL COMPARTMENTS

The vertical exchange of a chemical substance between two vertically adjacent soil compartments occurs through advection and diffusion. Only the net advection in the downward direction is considered due to long-term infiltration of rain water. This percolation occurs only in the downward direction, and not laterally. Diffusion in the current TRIM.FaTE library is represented in both an upward and downward direction, but not horizontally. The focus is on vertical diffusion because it is assumed that the vertical transport of chemicals in soils exceeds the horizontal transport when the major source of contamination is from the air.

5.3.4.1 Vertical Diffusive Transfers

According to Equation 5-1, the concentration in each soil compartment i is given by:

$$C_{Si}(x) = C_{Si}(0) \exp(-\gamma_{Si}x) \quad (\text{same as Eq. 5-1})$$

where:

x	=	distance into the soil compartment measured from the top of the soil column (m);
$C_{Si}(0)$	=	peak chemical concentration in soil compartment i (g[chemical]/m ³ [soil]), which is related to the total inventory N_{Si} (g[chemical]) in this soil compartment (this relationship is provided below in Equation 5-30); and
γ_{Si}	=	the gradient of soil concentration change in soil compartment i (/m), which is obtained from the inverse of the normalized or characteristic depth X^* , which is $\gamma_{Si} = 1/X^*$.

Thus, the diffusive flow at the lower boundary of soil compartment i to compartment j is given by:

$$Diffusion\ Flow = -A_{Sij} \times De_{Si} \times \left. \frac{dC}{dx} \right|_{d_{Si}} = A_{Sij} \times De_{Si} \times C_{Si}(0) \times \gamma_{Si} \times e^{-\gamma_{Si} \times d_{Si}} \quad (Eq. 5-26)$$

where:

Diffusion Flow = movement of chemical mass from soil compartment *i* to *j*
(g[chemical]/day);
 A_{Sij} = area of interface between soil compartments *i* and *j* (m²[interface]);
 De_{Si} = effective diffusion coefficient in soil compartment *i* (m²/day);
 γ_{Si} = the gradient of soil concentration change in soil compartment *i* (/m); and
 d_{Si} = the thickness of soil compartment *i* (m).

Conservation of mass requires that the flow specified by Equation 5-26 out of soil compartment *i* must equal the flow into soil compartment *j* at the upper boundary of compartment *j*, that is:

$$Diffusion\ Flow = -A_{Sij} \times De_{Sj} \left. \frac{dC}{dx} \right|_0 = A_{Sij} \times De_{Sj} \times C_{Sj}(0) \times \gamma_{Sj} \quad (Eq. 5-27)$$

where:

De_{Sj} = effective diffusion coefficient in soil compartment *ji* (m²/day);
 γ_{Sj} = the gradient of soil concentration change in soil compartment *j* (/m); and
 d_{Sj} = the thickness of soil compartment *j* (m).

Combining Equations 5-26 and 5-27 gives:

$$Diffusion\ Flow = A_{Sij} \times \frac{\left[De_{Si} \times C_{Si}(0) \times \gamma_{Si} \times e^{-\gamma_{Si} \times d_{Si}} + De_{Sj} \times C_{Sj}(0) \times \gamma_{Sj} \right]}{2} \quad (Eq. 5-28)$$

$C_{Si}(0)$ is found from the condition:

$$N_{Si} = A_{Sij} \times \int_0^{d_{Si}} C_{Si}(0) \times e^{-\gamma_{Si} x} dx = A_{Sij} \times \frac{C_{Si}(0)}{\gamma_{Si}} \times (1 - e^{-\gamma_{Si} \times d_{Si}}) \quad (Eq. 5-29)$$

where:

N_{Si} = total chemical inventory in soil compartment *i* (g[chemical]).

Rearranging gives:

$$C_{Si}(0) = \frac{N_{Si} \times \gamma_{Si}}{A_{Sij} \times (1 - e^{-\gamma_{Si} \times d_{Si}})} \quad (\text{Eq. 5-30})$$

In order to conserve concentration equilibrium at the boundary between two soil compartments, the following condition must hold:

$$C_{Sj}(0) = \frac{Z_{Total_Sj}}{Z_{Total_Si}} \times C_{Si}(0) \times e^{-\gamma_{Si} d_{Si}} = \frac{Z_{Total_Sj}}{Z_{Total_Si}} \times \frac{N_{Si} \times \gamma_{Si} \times e^{-\gamma_{Si} \times d_{Si}}}{A_{Sij} \times (1 - e^{-\gamma_{Si} \times d_{Si}})} \quad (\text{Eq. 5-31})$$

where:

Z_{Total_Sj} = total fugacity capacity of the chemical in soil compartment j (mol/m³-Pa); and
 Z_{Total_Si} = total fugacity capacity of the chemical in soil compartment i (mol/m³-Pa).

Substituting Equations 5-30 and 5-31 into Equation 5-28 gives:

$$\text{Diffusion Flow} = \frac{N_{Si} \times \gamma_{Si}}{Z_{Total_Si} \times (e^{+\gamma_{Si} \times d_{Si}} - 1)} \times \left(\frac{De_{Si} \times \gamma_{Si} \times Z_{Total_Si} + De_{Sj} \times \gamma_{Sj} \times Z_{Total_Sj}}{2} \right) \quad (\text{Eq. 5-32})$$

Then in order to express mass transfer between two compartments, the diffusion flow is represented in the following form:

$$\text{Diffusion Flow} = A_{Sij} \times Y_{Sij} \times \left(\frac{N_{Si}}{Z_{Total_Si} \times V_{Si}} - \frac{N_{Sj}}{Z_{Total_Sj} \times V_{Sj}} \right) \quad (\text{Eq. 5-33})$$

where:

N_{Sj} = the total chemical inventory in soil compartment j (g[chemical]);
 V_{Si} = volume of soil compartment i (m³);
 V_{Sj} = volume of soil compartment j (m³); and
 Y_{Sij} = fugacity-capacity adjusted mass transfer coefficient between soil compartments i and j , mol/(m²-Pa-day).

The total chemical inventory, N_{Sj} , in soil compartment j , is given by:

$$N_{Sj} = A_{Sj} \times \int_0^{d_{Sj}} C_{Sj}(0) \times e^{-\gamma_{Sj} x} dx = A_{Sj} \times \frac{C_{Sj}(0)}{\gamma_{Sj}} \times (1 - e^{-\gamma_{Sj} \times d_{Sj}}) \quad (\text{Eq. 5-34})$$

Substituting Equation 5-31 in Equation 5-34 gives:

$$N_{Sj} = \frac{Z_{Total_Sj} \times N_{Si} \times \gamma_{Si} \times (1 - e^{-\gamma_{Si} \times d_{Si}})}{Z_{Total_Si} \times \gamma_{Sj} \times (e^{+\gamma_{Si} \times d_{Si}} - 1)} \quad (\text{Eq. 5-35})$$

An expression for Y_{Sij} is obtained by substituting Equation 5-35 for N_{Sj} in Equation 5-33 and then setting Equation 5-33 equal to Equation 5-32:

$$\frac{N_{Si} \times \gamma_{Si}}{Z_{Total_Si} \times (e^{+\gamma_{Si} \times d_{Si}} - 1)} \times \left(\frac{De_{Si} \times \gamma_{Si} \times Z_{Total_Si} + De_{Sj} \times \gamma_{Sj} \times Z_{Total_Sj}}{2} \right) =$$

$$Y_{Sij} \times \frac{N_{Si}}{Z_{Total_Si}} \times \left(\frac{1}{d_{Si}} - \frac{\gamma_{Si} \times (1 - e^{-\gamma_{Sj} \times d_{Sj}})}{d_{Sj} \times \gamma_{Sj} \times (e^{+\gamma_{Si} \times d_{Si}} - 1)} \right) \quad (\text{Eq. 5-36})$$

Rearranging gives:

$$Y_{Sij} = \frac{(Z_{Total_Si} \times De_{Si} \times \gamma_{Si}) + (Z_{Total_Sj} \times De_{Sj} \times \gamma_{Sj})}{2 \times \left[\frac{(e^{+\gamma_{Si} \times d_{Si}} - 1)}{\gamma_{Si} \times d_{Si}} - \frac{(1 - e^{-\gamma_{Si} \times d_{Si}})}{\gamma_{Sj} \times d_{Sj}} \right]} \quad (\text{Eq. 5-37})$$

The definition of Y_{Sij} in Equation 5-37 completes the definition of all terms in Equation 5-33.

For the diffusive transfer of chemical from the higher soil compartment i (e.g., root-zone soil) to the soil compartment j below (e.g., vadose-zone soil), the transfer factor can be calculated as follows:

$$T_{Si \rightarrow Sj}^{dif} = \frac{Y_{Sij}}{d_{Si} \times Z_{Total_Si}} \quad (\text{TF 5-7})$$

For the diffusive transfer of chemical from the lower soil compartment j (e.g., vadose-zone soil) to the soil compartment i above (e.g., root-zone soil), the transfer factor can be calculated as follows:

$$T_{Sj \rightarrow Si}^{dif} = \frac{Y_{Sij}}{d_{Sj} \times Z_{Total_Sj}} \quad (\text{TF 5-8})$$

Note that both TF 5-7 and TF 5-8 assume that the normalized depth of the higher soil compartment i is thinner than the lower soil compartment j (i.e., $d_{Si} \times \gamma_{Si} < d_{Sj} \times \gamma_{Sj}$). The variable γ_{Si} , the soil penetration gradient (/m), is used to normalize depth in each soil compartment as shown above.

5.3.4.2 Downward Advective Transfer (Percolation)

The advection flow (i.e., percolation) from soil compartment i to j at the lower end, d_i , of compartment i is given by:

$$Advection\ Flow(Si \rightarrow Sj) = A_{Sij} \times ve_i \times C_{Si}(0) \exp(-\gamma_{Si} \times d_{Si}) \quad (\text{Eq. 5-38})$$

where:

Advection Flow = movement of chemical mass from soil compartment *i* to *j* (g[chemical]/day);
 ve_i = the effective advection velocity of a chemical in the soil compartment *i* (m/day), which is equal to the rate of soil-solution movement, v_i , multiplied by the fugacity capacity of the moving phase and divided by the total fugacity capacity of soil compartment *i*:

$$ve_i = \frac{v_i \times Z_{pure_water}}{Z_{Total_Si}} \quad (\text{Eq. 5-39})$$

where:

v_i = the average downward velocity of the moving phase (assumed to be water) in the soil compartment *i* (m/day).

Substituting Equation 5-30 for $C_i(0)$ in Equation 5-38 gives:

$$\frac{dN_{Sj}}{dt} = \frac{N_{Si} \times \gamma_{Si} \times ve_i}{(e^{+\gamma_{Si} \times d_{Si}} - 1)} \quad (\text{Eq. 5-40})$$

where:

N_{Sj} = chemical inventory in soil compartment *j* (g[chemical]); and
 N_{Si} = chemical inventory in soil compartment *i* (g[chemical]).

From this equation, we can derive terms for the advective transfer of chemical downward from soil compartment *i* to soil compartment *j* below as:

$$T_{Si \rightarrow Sj}^{perc} = \frac{ve_i \times \gamma_{Si}}{(e^{+\gamma_{Si} \times d_{Si}} - 1)} \quad (\text{TF 5-9})$$

5.4 STORM-WATER RUNOFF ALGORITHMS

Horizontal transport processes included in TRIM.FaTE include runoff (Section 5.4.1) and erosion (Section 5.4.2) due to rainfall.

5.4.1 AQUEOUS-PHASE TRANSPORT PROCESSES

During a rainfall event, some of the water travels laterally across the soil as runoff. As the water travels over the soil, the concentration of the water approaches that of the soil pore water beneath it. Although the water flowing over the soil does not necessarily reach

equilibrium instantaneously, some researchers use an approximation that runoff is in equilibrium with the soil pore water (Wallach et al. 1989). Currently in TRIM.FaTE, an equilibrium relationship between the runoff water and the soil pore water is used. Runoff water is considered a phase of the surface soil compartment at each spatial location. A mass-balance approach is used to determine the concentration in runoff water that moves from one surface soil compartment to a horizontally adjacent compartment.

Runoff transport is assumed to carry chemical from the surface soil compartment of one land unit to the next. During a rain event the surface soil compartment is assumed to be saturated with rain water and this water is assumed to be in equilibrium with the soil solids on the surface. It should be recognized that at times (*e.g.*, short rain events, during very dry periods of the year) the soil will not necessarily be fully saturated with rain water. However, the assumption of saturation by rain is not expected to have a large impact on results for events when the soil is not saturated. Moreover, a lack of information on the extent to which soil is saturated during rain makes this a convenient starting point. The assumption of chemical equilibrium between the surface soil water and surface soil solids has more uncertainty and needs further research.

During periods of no rain, the total fugacity capacity of the i^{th} surface soil compartment, Z_{Total_Ssi} is given by:

$$Z_{Total_Ssi} = \epsilon \times Z_{pure_air} + \theta \times Z_{pure_water} + (1 - \phi) \times Z_{pure_solid} \quad (\text{Eq. 5-41})$$

During periods of rain, when the soil becomes saturated with water, we account for the different composition of the soil by writing the fugacity capacity of the chemical in the surface soil compartment as follows:

$$Z_{Total_Ssi} = [(Rh + \phi \times d_{Ssi}) \times Z_{pure_water} + (1 - \phi \times d_{Ssi}) \times Z_{pure_solid}] \times d_{Ssi} \quad (\text{Eq. 5-42})$$

where:

- Z_{Total_Ssi} = total fugacity capacity of the chemical in the i^{th} surface soil compartment (mol/m³-Pa);
- Z_{pure_air} = fugacity capacity of chemical in air (excluding suspended particles) (mol/m³-Pa);
- Z_{pure_water} = fugacity capacity of chemical in water (excluding suspended sediments) (mol/m³-Pa);
- Z_{pure_solid} = fugacity capacity of the chemical in solid phase in the surface soil compartment (mol/m³-Pa);
- ϵ = volume fraction of the surface soil compartment that is gas (unitless);
- θ = volume fraction of the surface soil compartment that is water (unitless);
- ϕ = total void fraction (or porosity) in surface soil, $\phi = \epsilon + \theta$ (unitless);
- Rh = hydraulic radius of the water flowing over the surface soil during a rain event (m); and
- d_{Ssi} = depth of the surface soil compartment (m).

The hydraulic radius, Rh , for flow of water on top of the soil surface is site specific and depends on the hydraulic gradient (slope of the flow), the rainfall rate, and the recharge rate. It is considered an uncertain variable. A hydraulic balance is needed to determine the flow of the water and the depth of the runoff stream. From the Geographic Information System (GIS) data, the runoff is estimated.

Although runoff occurs only during rain events, in the current TRIM.FaTE library, it is modeled as a continuous process based on an annual average runoff value divided by 365 days. The horizontal advective flow of chemical in water from surface soil compartment i to adjacent compartment j is given by:

$$\text{Runoff Flow } (S_{si} \rightarrow S_{sj}) = \frac{\text{runoff} \times f_{\text{runoff}}(S_{si} \rightarrow S_{sj}) \times f_{\text{avail_runoff}} \times Z_{\text{pure_water}}}{Z_{\text{Total_}S_{si}} \times d_{S_{si}}} \times N_{S_{si}} \quad (\text{Eq. 5-43})$$

where:

$$\begin{aligned} \text{Runoff Flow } (S_{si} \rightarrow S_{sj}) &= \text{average daily horizontal transfer of chemical carried in surface soil pore water down-gradient from surface soil compartment } i \text{ to surface soil compartment } j \text{ (g[chemical]/day);} \\ \text{runoff} &= \text{aerial flux of water that is transported away from surface soil compartment } i \text{ (m}^3\text{[water]/m}^2\text{[surface soil]-day);} \\ f_{\text{runoff}}(S_{si} \rightarrow S_{sj}) &= \text{fraction of water that runs off of surface soil compartment } i \text{ that is transported to compartment } j \text{ (unitless);} \\ f_{\text{avail_runoff}} &= \text{fraction of surface soil compartment } i \text{ that is available for runoff (unitless);} \\ Z_{\text{Total_}S_{si}} &= \text{total fugacity capacity of the chemical in the } i^{\text{th}} \text{ surface soil compartment (mol/m}^3\text{-Pa) as determined in Equation 5-42;} \\ Z_{\text{pure_water}} &= \text{fugacity capacity of chemical in water (excluding suspended sediments) (mol/m}^3\text{-Pa); and} \\ N_{S_{si}} &= \text{total chemical inventory in the surface soil compartment } i \text{ (g[chemical]).} \end{aligned}$$

Using substitutions for $1/d_{S_{si}}$ and $Z_{\text{pure_water}}/Z_{\text{Total_}S_{si}}$ as indicated below, Equation 5-43 is equivalent to:

$$\frac{dN_{S_{sj}}}{dt} = \text{runoff} \times f_{\text{runoff}}(S_{si} \rightarrow S_{sj}) \times f_{\text{avail_runoff}} \times \frac{A_{S_{si}}}{V_{S_{si}}} \times f_{ML} \times N_{S_{si}} \quad (\text{Eq. 5-44})$$

where:

$$1/d_{S_{si}} = A_{S_{si}}/V_{S_{si}} \text{ (m), i.e., the area of surface soil compartment } i \text{ (m}^2\text{) divided by the volume of the surface soil compartment } i \text{ (m}^3\text{);}$$

and:

$$\frac{Z_{pure_water}}{Z_{Total_Ssi}} = \frac{Mass_Fraction_Dissolved}{Volume_Fraction_Liquid} = f_{ML} \quad (\text{Eq. 5-45})$$

as described in Chapter 2, Equation 2-80 (*i.e.*, f_{ML} equals the fraction of the mass of total chemical in surface soil compartment i that is dissolved in water divided by the volume fraction of the surface soil compartment that is liquid (water)) (unitless).

From Equation 5-44, the expression for $T_{Ssi \rightarrow Ssj}(runoff)$ that is in the TRIM.FaTE library can be obtained:

$$T_{Ssi \rightarrow Ssj}^{runoff} = runoff \times f_{runoff}(Ssi \rightarrow Ssj) \times f_{avail_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \quad (\text{TF 5-10a})$$

$$T_{Ssi \rightarrow SW}^{runoff} = runoff \times f_{runoff}(Ssi \rightarrow SW) \times f_{avail_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \quad (\text{TF 5-10b})$$

Runoff from a surface soil compartment might flow into an adjacent to a surface water (SW) body. The equation for that transfer is the same as for runoff to an adjacent surface soil compartment, except that the receiving compartment is the surface water compartment instead:

Finally, for a surface soil compartment adjacent to the boundary of the modeling region, runoff from the compartment can move out of the modeling region, which is modeled as a transfer to the surface soil sink (Ss_sink). The equation for runoff to a surface soil sink is similar to the previous equation:

$$T_{Ssi \rightarrow Ss_sink}^{runoff} = runoff \times f_{runoff}(Ssi \rightarrow Ss_sink) \times f_{avail_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \quad (\text{TF 5-10c})$$

It is possible for all three of these different runoff algorithms to apply to a given surface soil compartment i . The sum of the f_{runoff} values across all of the runoff algorithms applied to the same surface soil compartment cannot exceed 1.0.

5.4.2 SOLID-PHASE TRANSPORT PROCESSES

The algorithm for erosion runoff is based on knowledge of the erosion factor for the region being modeled. Similar to solution runoff, erosion is also applied only to the surface soil layer. Although erosion is most likely to occur during rain events, erosion can be modeled as a continuous event. The flow of chemical (mol/d) from one surface soil compartment to another by erosion is represented by the following expression:

$$Erosion\ Flow(Ssi \rightarrow Ssj) = \frac{erosion \times f_{erosion}(Ssi \rightarrow Ssj) \times f_{avail_erosion} \times Z_{pure_solid} \times N_{Ssi}}{Z_{Total_Ssi} \times \rho_P \times d_{Ssi}} \quad (\text{Eq. 5-46})$$

where:

$$\begin{aligned}
 \text{Erosion Flow } (S_{si} \rightarrow S_{sj}) &= \text{average daily horizontal transfer of chemical carried in} \\
 &\quad \text{surface soil particles down-gradient from surface soil} \\
 &\quad \text{compartment } i \text{ to surface soil compartment } j \\
 &\quad \text{(g[chemical]/day);} \\
 \text{erosion} &= \text{erosion factor (kg[soil solids]/m}^2\text{[surface soil]-day);} \\
 f_{\text{erosion}}(S_{si} \rightarrow S_{sj}) &= \text{fraction of soil eroded from surface soil compartment } i \text{ that is} \\
 &\quad \text{transported to surface soil compartment } j \text{ (unitless);} \\
 f_{\text{avail_erosion}} &= \text{fraction of surface soil compartment } i \text{ that is available for erosion} \\
 &\quad \text{(e.g., not paved or otherwise covered by non-soil surfaces);} \\
 Z_{\text{pure_solid}} &= \text{fugacity capacity of chemical in the solid phase in the } i^{\text{th}} \text{ surface} \\
 &\quad \text{soil compartment (mol/m}^3\text{-Pa);} \\
 Z_{\text{Total_Ssi}} &= \text{total fugacity capacity of chemical in the } i^{\text{th}} \text{ surface soil compartment} \\
 &\quad \text{(mol/m}^3\text{-Pa);} \\
 \rho_P &= \text{density of the soil particles (kg[particles]/m}^3\text{[particles]);} \\
 d_{Ssi} &= \text{depth of the surface soil compartment (m); and} \\
 N_{Ssi} &= \text{the total chemical inventory in soil compartment } i \text{ (g[chemical])}.
 \end{aligned}$$

Substituting for $1/d_{Ssi}$ and $Z_{\text{pure_solid}}/Z_{\text{Total_Ssi}}$ as indicated below, Equation 5-46 is equivalent to:

$$\frac{dN_{Ssj}}{dt} = \text{erosion} \times f_{\text{erosion}}(S_{si} \rightarrow S_{sj}) \times f_{\text{avail_erosion}} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \times N_{Ssi} \quad (\text{Eq.5-47})$$

where:

$$\begin{aligned}
 1/d_{Ssi} &= A_{Ssi}/V_{Ssi} \text{ (m);} \\
 A_{Ssi} &= \text{area of surface soil compartment } i \text{ (m}^2\text{);} \\
 V_{Ssi} &= \text{volume of the surface soil compartment } i \text{ (m}^3\text{);}
 \end{aligned}$$

and:

$$f_{MS} = \frac{Z_{\text{pure_solid}}}{Z_{\text{Total_Air}}} = \frac{\text{Mass_Fraction_Sorbed}}{\text{Volume_Fraction_Solid}} \quad (\text{same as Eq. 5-23})$$

as described in Chapter 2, Equation 2-79 (i.e., fraction of the mass of total chemical in surface soil compartment i that is sorbed to solid particles divided by the volume fraction of the surface soil compartment that is solid particles) (unitless).

From Equation 5-47, the expression for $T_{Ssi \rightarrow Ssj}(\text{erosion})$ can be obtained:

$$T_{Ssi \rightarrow Ssj}^{\text{erosion}} = \text{erosion} \times f_{\text{erosion}}(S_{si} \rightarrow S_{sj}) \times f_{\text{avail_erosion}} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \quad (\text{TF 5-11a})$$

Erosion from a surface soil compartment might flow into an adjacent to a surface water body. The equation for that transfer is the same as for erosion to an adjacent surface soil compartment, except that the receiving compartment is the surface water body instead:

$$T_{Ssi \rightarrow SW}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow SW) \times f_{avail_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \quad (TF\ 5-11b)$$

Finally, for a surface soil compartment adjacent to the boundary of the modeling region, erosion from the compartment can move out of the modeling region, which is modeled as a transfer to the surface soil sink (Ss_sink). The equation for erosion to a surface soil sink is similar to the previous equation:

$$T_{Ssi \rightarrow SW}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow SW) \times f_{avail_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \quad (TF\ 5-11c)$$

It is possible for all three of these different erosion algorithms to apply to a given surface soil compartment i . The sum of the $f_{erosion}$ values across all of the erosion algorithms applied to the same surface soil compartment cannot exceed 1.0.

5.5 GROUND-WATER ALGORITHMS

The horizontal flow of pollutants in the saturated zone (ground water) is not expected to be a significant pathway when considering air pollutants. Downward advective transport from the vadose zone to ground water has been simulated because it is a more significant process than diffusion/dispersion. However, the relative importance of diffusive/dispersive transfer compared with advective transport between the vadose zone and the ground-water zone needs to be investigated further.

In the current version of TRIM.FaTE, ground water is modeled as a receiving compartment for percolation from the vadose zone. The same equation used to estimate the transfer of chemical via percolation from one soil compartment to another soil compartment immediately below it (*i.e.*, TF 5-9) is used to estimate the transfer factor for percolation from the vadose-zone soil (Sv) compartment to ground water (GW):

$$T_{Sv \rightarrow GW} = \frac{ve_{Sv} \times \gamma_{Sv}}{(e^{+\gamma_{Sv} \times d_{Sv}} - 1)} \quad (TF\ 5-12)$$

where:

$T_{Sv \rightarrow GW}$ = transfer factor from vadose-zone soil to ground water (/day);
 ve_{Sv} = the effective advection velocity of a chemical in the vadose-zone soil compartment (m/day), which is equal to the rate of soil-solution movement, v_i , multiplied by the fugacity capacity of the moving phase

(water) and divided by the total fugacity capacity of the vadose-zone soil compartment;
 γ_{Sv} = the gradient of soil concentration change in the vadose-zone soil compartment (/m); and
 d_{Sv} = thickness of vadose-zone soil compartment (m).

The transfer factor from ground water to surface water is based on aqueous-phase advection only. It can be calculated as:
 where:

$T_{GW \rightarrow SW}$ = transfer factor from ground-water to surface-water compartments (/day);
 $A_{SWG W}$ = interfacial area between the surface-water and ground-water compartments (m^2);
 V_{GW} = volume of the ground-water compartment (m^3);
 Z_{pure_water} = fugacity capacity of the chemical in pure water (mol/m^3 -Pa);
 Z_{Total_GW} = total fugacity capacity of the chemical in the ground-water compartment (mol/m^3 -Pa);
 $recharge$ = annual average daily recharge from ground water into surface water (m/day); and

$$T_{GW \rightarrow SW} = \frac{A_{SWG W}}{V_{GW}} \times \frac{Z_{pure_water}}{Z_{Total_GW}} \times recharge \quad (TF\ 5-13a)$$

$$= \frac{A_{SWG W}}{V_{GW}} \times f_{ML} \times recharge \quad (TF\ 5-13b)$$

f_{ML} = $Z_{pure_water}/Z_{Total-GW}$, which equals *Mass_Fraction_Dissolved / Volume_Fraction_Liquid* (i.e., fraction of the mass of total chemical in the ground-water compartment that is dissolved in water divided by the volume fraction of the ground-water compartment that is liquid water, see Equations 2-72 and 2-80) (unitless).

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